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Gradient Systems

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In the space of vectors $x = (x_1, x_2, \ldots, x_N)$, we consider an arbitrary scalar function (Hamiltonian) $h = h(x)$ and an arbitrary matrix $M = (M_{ki})$ with constant elements. The system of equations

$$\frac{dx_i}{dt} = M\left(\frac{dh}{dx_i}\right)^* \quad (1)$$

is called a gradient system. In [2], similar systems were first examined under the assumption that M is nonsingular, and they were called symmetrizable. The star converts a row into a column and is required for matching the tensor dimensions on the left- and right-hand sides of the system. In the special case of M satisfying $M^2 = -E$ (the dimension of the phase space is even: $\dim x = 2s$), a Hamiltonian system arises.

PAIRWISE INTERACTION

Consider a macroscopic system consisting of a large number N^2 of identical components x_i (where $N^2 \gg 1$) and assume that the equations of motion of the system are given by a Hamiltonian H and a matrix M:

$$H = H(x_1, x_2, \ldots, x_N), \quad \frac{dx_i}{dt} = M\left(\frac{\partial H}{\partial x_i}\right)^*. \quad (2)$$

Usually, we deal with the pairwise interaction

$$H = \sum_{i=1}^{N}\sum_{l=1}^{N} H(x_i, x_l),$$

where H is the sum of N^2 Hamiltonians $H = H(x,y)$ defining the interaction of the two components x and y. The terms differ from one another only by the argument indices.

KHINCHIN SUMMATORY FUNCTIONS

A systematic study of the properties of summatory functions in statistics goes back to Khinchin's work [1] and is associated with the generalization of the law of large numbers to functions, although the role of symmetric functions was already well known in algebra [e.g., Viète's formulas (about 1590)]. In our problem, summatory functions arise by themselves from the application of Fourier series expansions of functions in terms of a basis.

Consider an arbitrary basis $\{z_\alpha(x)\}$ in the space of functions of one variable x. The interaction Hamiltonian $H(x, y)$ is expanded in terms of the corresponding basis $\{z_\alpha(x)z_\beta(y)\}$ in the space of functions of the two variables:

$$H(x, y) = \sum_{\alpha\beta} H^{\alpha\beta} z_\alpha(x) z_\beta(y). \quad (3)$$

Substituting the resulting expression into the Hamiltonian of the system yields

$$H = \sum_{\alpha\beta} H^{\alpha\beta}\left[\sum_l z_\alpha(x_l)\right]\left[\sum_l z_\beta(x_l)\right]. \quad (4)$$

Thus, the summatory functions $Z_\alpha = \sum_{i=l}^{N} z_\alpha(x_i)$ arise automatically on changing the order of summatory. Expressing H in terms of the new variables Z_α,

$$H = \sum_{\alpha\beta} H^{\alpha\beta} Z_\alpha Z_\beta, \quad (5)$$

we arrive at an important conclusion: the Hamiltonian is a quadratic function of the macroscopic variables Z_α (the function is quadratic because the interaction is pairwise). In addition, note that the coefficients of the quadratic form H coincide with the Fourier coefficients $H^{\alpha\beta}$ in the expansion of $H(x, y)$ in terms of $\{z_\alpha(x)z_\beta(y)\}$.

MACRODYNAMICS

Writing the Hamiltonian H of the system in terms of the variables Z $H = H(Z)$ simplifies the equations of motion to

$$\frac{dx_i}{dt} = \sum_\beta \frac{\partial H}{\partial Z_\beta} M \frac{\partial z_\beta}{\partial x_i}. \quad (6)$$

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The right-hand sides of the resulting equations contain both scalar (macroscopic) quantities,

$$L^{\beta} = \frac{\partial H}{\partial Z_{\beta}}, \tag{7}$$

and vector (microscopic) fields,

$$a_{\beta}(x) = M\left(\frac{\partial z_{\beta}}{\partial x}\right)^{*}. \tag{8}$$

In this notation, we can more easily see the structure of the equations of motion

$$\frac{dx_i}{dt} = \sum_{\beta} L^{\beta} a_{\beta}(x_i),$$

which prompts the idea of extracting macrodynamics (the evolution of Z_{β}) from the huge set ($N \gg 1$) of microscopic motions x_i.

Differentiating the relation defining Z_{α} with respect to time,

$$\frac{dZ_{\alpha}}{dt} = \sum_{i} \frac{\partial z_{\alpha}}{\partial x_i}\frac{dx_i}{dt}, \tag{9}$$

and substituting the derivatives of x_i, we obtain

$$a_{\beta}(x_i) = M\left(\frac{\partial z_{\beta}}{\partial x_i}\right)^{*},$$

$$\frac{dZ_{\alpha}}{dt} = \sum_{i} \frac{\partial z_{\alpha}}{\partial x_i}\left[\sum_{\beta} L^{\beta} a_{\beta}(x_i)\right] = \sum_{\beta} L^{\beta}\left\{\sum_{i} \frac{\partial z_{\alpha}}{\partial x_i} M\left(\frac{\partial z_{\beta}}{\partial x_i}\right)^{*}\right\}. \tag{10}$$

The expression in curly brackets is a summatory function, and each of its terms can be expanded in terms of a basis:

$$\frac{\partial z_{\alpha}}{\partial x} M\left(\frac{\partial z_{\beta}}{\partial x_i}\right) = I^{\gamma}_{\alpha\beta} z_{\gamma}(x_i).$$

Here, $I^{\gamma}_{\alpha\beta}$ are constants (Fourier coefficients) determined only by the properties of $\{z_{\alpha}(x)\}$ and M but not related in any way to the original equations. Summing the equations over all the components x_i, we entirely eliminate the μ variables and obtain the equations

$$\frac{dZ_{\alpha}}{dt} = I^{\gamma}_{\alpha\beta} Z_{\gamma} L^{\beta}. \tag{11}$$

Substituting L^{β} from (7) gives the macrodynamic equations

$$\frac{dZ_{\alpha}}{dt} = I^{\gamma}_{\alpha\beta} Z_{\gamma} \frac{\partial H}{\partial Z_{\beta}}. \tag{12}$$

M-ALGEBRAS AND QUADRATIC POLYNOMIALS

The analysis above lacks formal rigor, since we ignored the convergence of the arising series. However, these calculations become strict for the important case of M-algebras.

Definition. A finite-dimensional subspace of a space of functions with a basis $z_{\gamma}(x)$ is called an M-algebra if it is closed under the ⊗ product operation defined as

$$z_{\alpha} \otimes z_{\beta} = \frac{dz_{\alpha}}{dx} M\left(\frac{dz_{\beta}}{dx}\right) = I^{\gamma}_{\alpha\beta} z_{\gamma}(x). \tag{13}$$

The expansion coefficients $I^{\gamma}_{\alpha\beta}$ are called the structural constants of the algebra.

The nonemptiness of the set of defined objects is an obvious requirement for the definition to be meaningful. In our case, the space of quadratic forms constitutes an algebra for any matrix M. This follows from the fact that the derivative (gradient) of a quadratic form is a linear form and that the product of two such forms is again a quadratic form. The M-algebra can be expanded by adding a constant and all the linear functions x_i. The example of the expanded M-algebra demonstrates the nonemptiness of the sets of M-algebras but does not exhaust this set. In the simplest case of a system with one degree of freedom, a finite algebra is generated only by the two functions

$$a(x) = x, \quad b(x) = \frac{x^2}{2}. \tag{14}$$

Even in this case, we have a meaningful problem. Let

$$H = H(A, B), \quad \text{where} \quad A = \sum_{i} x_i, \quad B = \sum_{i} \frac{x_i^2}{2}.$$

In the new notation, the equations for x_i take the form

$$\frac{dx_i}{dt} = \frac{\partial H}{\partial A} + x_i \frac{\partial H}{\partial B}. \tag{15}$$

From (15), we can derive the following macrodynamic equations, which close the system:

$$\begin{aligned} \frac{dA}{dt} &= N\frac{\partial H}{\partial A} + A\frac{\partial H}{\partial B}, \\ \frac{dB}{dt} &= A\frac{\partial H}{\partial A} + 2B\frac{\partial H}{\partial B}. \end{aligned} \tag{16}$$

In these equations, the assumption that the interaction is pairwise and, hence, the Hamiltonian H is quadratic with respect to the M-variables A and B has not been applied. The equations are valid under the much more general assumption

$$H = H(A, B). \tag{17}$$

Note that all the equations in (13) coincide (up to the notation) with the equation for the μ-motion of a single component:

$$\frac{dx}{dt} = \frac{\partial H}{\partial A} + x\frac{\partial H}{\partial B}. \tag{18}$$

Therefore, the system of N equations is, in fact, reduced to the system of three equations in (15) and (16). By (analytically or numerically) integrating system (16), we obtain one linear equation (18) with variable coefficients. Any solution $x_i(t)$ is obtained by substituting appropriate initial data into the solution to Eq. (14).

In the two-dimensional case [$x = (p, q)$], there are five M-variables (from the algebra of quadratic polynomials):

$$P = \sum p_i, \quad W = \sum \frac{p_i^2}{2}, \quad R = \sum p_i q_i, \qquad Q = \sum q_i, \quad Z = \sum \frac{q_i^2}{2}. \tag{19}$$

If the Hamiltonian is a function of only macroscopic variables [i.e., $H = H(P, Q, R, W, Z)$], the Hamilton system

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial p_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$$

can be rewritten as

$$\begin{aligned} \frac{dp_i}{dt} &= -\frac{\partial H}{\partial Q} - p_i\frac{\partial H}{\partial R} - q_i\frac{\partial H}{\partial Z}, \\ \frac{dq_i}{dt} &= \frac{\partial H}{\partial p} + p_i\frac{\partial H}{\partial W} + q_i\frac{\partial H}{\partial R}. \end{aligned} \tag{20}$$

This yields the macrodynamic equations

$$\begin{aligned} \frac{dP}{dt} &= -N\frac{\partial H}{\partial Q} - P\frac{\partial H}{\partial R} - Q\frac{\partial H}{\partial Z}, \\ \frac{dQ}{dt} &= N\frac{\partial H}{\partial P} - P\frac{\partial H}{\partial W} - Q\frac{\partial H}{\partial R}, \\ \frac{dR}{dt} &= P\frac{\partial H}{\partial P} - 2W\frac{\partial H}{\partial R} - Q\frac{\partial H}{\partial Q} - 2Z\frac{\partial H}{\partial Z}, \\ \frac{dW}{dt} &= -P\frac{\partial H}{\partial Q} - 2W\frac{\partial H}{\partial R} - R\frac{\partial H}{\partial Z}, \\ \frac{dZ}{dt} &= Q\frac{\partial H}{\partial P} - R\frac{\partial H}{\partial W} + 2Z\frac{\partial H}{\partial R}. \end{aligned} \tag{21}$$

Of course, the mechanism involved in extracting macrodynamic equations is the same as in the case of a general M-algebra. Note the important special case of mechanical systems where the Hamiltonian is the sum of the kinetic and potential energies:

$$H = \sum_i \frac{p_i^2}{2Nm} + \sum_i \sum_l U\left(q_i, q_l, \frac{q_i^2}{2}, \frac{q_l^2}{2}\right). \tag{22}$$

Then,

$$H = \frac{1}{m}W + U(Q, Z), \tag{23}$$

and the system of macrodynamic equations considerably simplifies to

$$\begin{aligned} \frac{dP}{dt} &= -N\frac{\partial U}{\partial Q} - Q\frac{\partial U}{\partial Z}, \\ \frac{dQ}{dt} &= \frac{1}{m}P, \\ \frac{dR}{dt} &= \frac{2}{m}W - Q\frac{\partial U}{\partial Q} - 2Z\frac{\partial U}{\partial Z}, \\ \frac{dW}{dt} &= -P\frac{\partial U}{\partial Q} - R\frac{\partial U}{\partial Z}, \\ \frac{dZ}{dt} &= \frac{1}{m}R. \end{aligned} \tag{24}$$

An analysis of the behavior of the macrodynamic equations is beyond the scope of this work, but numerical experiments have revealed not only equilibrium states but also rather diverse (and intricate) steady-state regimes.

DECOUPLING OF COMPONENTS

Let us describe the basic ideas contained in the analysis. Suppose that we are given an arbitrary M-algebra $\{z_\gamma(x)\}$

$$\frac{dz_\alpha}{dx}M\left(\frac{dz_\beta}{dx}\right)^* = I_{\alpha\beta}^\gamma z_\gamma(x) \tag{25}$$

and a Hamiltonian $H = H(Z_1, Z_2, \ldots, Z_k)$, which is a function of only the macroscopic variables

$$Z_\alpha = \sum_i z_\alpha(x_i)$$

and (in the case of a pairwise interaction) is a quadratic polynomial in its arguments. The system $\{M, H\}$ generated by the matrix M and the Hamiltonian H,

$$\frac{dx_i}{dt} = M\left(\frac{\partial H}{\partial x_i}\right)^*, \tag{26}$$

can be written in the new variables as

$$\frac{dx_i}{dt} = \sum_\beta \left(\frac{\partial H}{\partial Z_\beta}\right) M\left(\frac{dz_\beta}{dx_i}\right)^*. \tag{27}$$

Macroscopic motions can be extracted from this system:

$$\frac{dZ_\alpha}{dt} = I^\gamma_{\alpha\beta} Z_\gamma \frac{\partial H}{\partial Z_\beta}. \qquad (28)$$

Moreover, given Z, the system of microscopic motions x_i splits into independent motions. All the equations are identical in form (up to the notation of the variables) to a single standard equation for x:

$$\frac{dx}{dt} = \frac{\partial H}{\partial Z_\alpha} M \left(\frac{dz_\alpha}{dx}\right)^*. \qquad (29)$$

Therefore, the trajectory of the system in the multidimensional macroscopic space $(x_1, x_2, \ldots, x_N)$ can be precisely replaced by the set of N trajectories (differing only in the initial data) in the standard μ-space of x.

The steps in the analysis can be described as follows. In the original system, each component interacts in a pairwise manner with the others. Altogether, there are N^2 couplings. On introducing the "superfluous" macroscopic variables Z, the interaction between x_i and x_k can be replaced by the action of Z on x_i. There remain N couplings. All the components are identical; therefore, motion in the multidimensional macroscopic space is equivalent to the motion of a cloud of points in the standard μ-space of x. Only one coupling remains in this case.

Knowledge of a single trajectory of the macroscopic system is sufficient for decoupling its components. Such a trajectory can easily be computed on a modern computer because the dimension of the macroscopic system is independent of N, although N can be involved in the coefficients of the macroscopic system.

EQUIVALENT FIELD AND MACRODYNAMIC EQUILIBRIUM

It is convenient to rewrite Eq. (29) as

$$\frac{dx}{dt} = M\left(\frac{\partial h}{\partial x}\right)^* \qquad (30)$$

by introducing an "equivalent" field $h(x, Z)$:

$$h(x, Z) = \sum_\alpha \frac{\partial H}{\partial Z_\alpha} z_\alpha(x). \qquad (31)$$

Then, the motion of x can be interpreted as motion in the "external" field $h(x, Z)$, whose parameters are determined by the macroscopic variables Z. An analysis of any system usually begins with the study of its steady-state regimes, and they are frequently the only objects of analysis if they are sufficient for practical purposes. Since the system of equations

$$\frac{dZ}{dt} = f(Z),$$

$$\frac{dx}{dt} = g(Z, x)$$

is "triangular" (i.e., the equation for Z does not involve x), we can introduce the concept of the macrodynamic equilibrium

$$f(Z) = 0, \quad Z = \text{const},$$

which means that only the macroscopic system is stationary. This is a natural generalization of the concept of a "thermodynamic equilibrium."

In a macroscopic equilibrium, the equivalent field $h(x, Z)$ is time-independent and the system of equations for x becomes autonomous. It is fairly likely that this important special case of the concept of an equivalent field corresponds to the concept of a self-consistent field in physics. However, a detailed analysis of this interesting question is beyond the scope of this paper. The stationary equivalent field is also interesting in that it provides a simple and visual interpretation of passage to the limit of $N \to \infty$. Each trajectory of the original system generates N trajectories in the space of the single component x. If the starting points of these trajectories are distributed sufficiently uniformly, the trajectories will fill (in the limit) the whole space. Therefore, the phase portrait of the system can be interpreted as the limit of the projection of a single trajectory of the original system onto the μ-space. This relation promises interesting results in future studies and considerably expands the applicability range of the qualitative theory of ordinary differential equations. Recall that the right-hand sides of the macrodynamic equations are always quadratic in the case of a pairwise interaction. This indicates a strong relationship between the systems under consideration and general bilinear systems [3].

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REFERENCES

1. A. Ya. Khinchin, *Mathematical Foundations of Statistical Mechanics* (Gostekhizdat, Moscow, 1943; Dover, New York, 1949).
2. A. M. Obukhov, Dokl. Akad. Nauk SSSR **233**, 35–38 (1977).
3. A. M. Molchanov, Preprint, ONTI NTsBI AN SSSR (1982).